

Analytic formulas for frequency and size dependence of absorption and scattering efficiencies of astronomical polycyclic aromatic hydrocarbons

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Abstract

In a series of two recent papers, the frequency and size distribution dependence of extinction spectra for astronomical silicate and graphite grains was analyzed by us in the context of MRN type interstellar dust models. These grains were taken to be homogeneous spheres following the power law ($a^{-3.5}$) size distribution which is very much in use. The analytic formulas were obtained for the graphite and silicate grains in wavelength range 1000Å - 22,500Å and their utility was demonstrated. In this paper of the series, we present analytic formulas for the scattering and absorption spectrum of another important constituent of interstellar dust models, namely, the polycyclic aromatic hydrocarbons (PAHs). Relative contribution of the PAHs to extinction *vis a vis* carbonaceous classical grains has been examined.

Keywords: Interstellar grains, Extinction spectrum, PAH, Size distribution dependence.

1 Introduction

In a recent series of two papers, we presented analytic formulas for the frequency and size distribution dependence of the extinction spectrum of astronomical silicate and graphite grains in the wavelength range 1000 Å - 22,500 Å [1,2] (hereafter referred to as RSG-1 and RSG-2). These formulas were worked out keeping in mind the two component interstellar dust models of Mathis, Rumble and Nordsieck (MRN) [3] type, wherein one assumes the dust grains to be a collection of bare silicate and graphite homogeneous spheres, each of the two components obeying a power law size distribution with exponent -3.5 , having a minimum radius (a_0) and a maximum radius (a_m). In our analysis, the admitted ranges of a_0 and a_m were $0.002 \mu m \leq a_0 \leq 0.005 \mu m$ and $0.15 \mu m \leq a_m \leq 0.25 \mu m$ for graphite grains and $0.004 \mu m \leq a_0 \leq 0.006 \mu m$ and $0.2 \mu m \leq a_m \leq 0.4 \mu m$ for silicate grains. These ranges are thought to be quite appropriate and allow one to have the kind of flexibility needed in fixing the values of a_0 and a_m . A comparison of extinction predicted by these formulas *vis-a-vis* exact Mie computations showed that these formulas give results which are in close proximity to exact computations. Hence, these formulas have the potential to be used efficiently for assessment of the extinction contributions of the silicate and graphite components in investigations and building of MRN type models without resorting to large scale numerical computations. Moreover, by selecting proper ranges of frequency, the extinction behavior can be effectively approximated by yet simpler forms (e.g., linear, quadratic, etc.). That is, further simplification can be made in an effort to set appropriate particle size ranges to start with. It may be mentioned here that analytic formulas fitting the extinction spectra of several stars have been obtained in the past by Cardelli *et al.* [4] and Fitzpatrick and Massa [5]. However, these parametrizations are mostly based on mathematical schemes. In contrast, the formulas provided in RSG-1 and RSG-2, give some degree of physical insight into the problem and also address the problem in terms of silicate and graphite grains separately with a provision of allowable variations in a_0 as well as in a_m - which are known to be quite adequate.

In the MRN type models it is generally assumed that carbonaceous grains have $a_0 \approx 0.005 \mu m$ and their optical properties are more like graphite grains. However, in more recent models it has been recognized that the carbonaceous component also has a sub-component of “very small grains” whose optical properties are different from that of graphite. These grains are the so-called polycyclic aromatic hydrocarbons that are referred to as “astronomical” PAHs in the literature.

1.1 Why PAH's

In 1956 Platt[6] proposed that very small grain or large molecules of radii around 10\AA to be present in the Interstellar Dust. Donn(1968)[7] proposed that polycyclic aromatic hydrocarbon like 'Platt Particles' may produce UV extinction in the interstellar spectra. Importance and ubiquity of polycyclic aromatic hydrocarbons is quite evident in literature addressing the interstellar extinction. The inclusion of PAH's is based on the three decades of research by various groups. The IR emission features are very well attributed to PAH's by now and also allow to place constraints on size distribution of very small dust components. Ubiquity of PAH's in many galaxies has been observationally verified by ISO and Spitzer, thus making Polycyclic Aromatic Hydrocarbons (PAH's) a very important constituents of Interstellar Dust(Draine and Li 2007,[8]). Draine and coworkers (Li and Draine 2001b[9], 2002a[10]; Weingartner and Draine 2001a[11]) proposed the Silicate- Graphite-PAH's model, of which PAH are the small-size end of the carbonaceous grains, is in excellent agreement with observations. For more details please refer to the paper by Li and Greenberg[12]. On these lines, in this paper, we aim at extending the analyses of RSG 1 and RSG 2 to include the extinction spectra analysis of the PAHs in the size range $5\text{\AA} \leq a \leq 50\text{\AA}$ and spectral domain 1000\AA to $22,500\text{\AA}$. The closed form analytic expressions for extinction by such grains should enable one to make more precise and elaborate model investigations and hence correct model building. The PAHs like grains can be further distinguished as being either in neutral or ionic state. Analytic formulas to evaluate and analyze the extinction spectrum have been obtained for both types of PAHs in this work. As the PAHs are very small in size, the scattering is expected to be unimportant [13]. Thus, the extinction can be effectively computed from the absorption only. However, for completeness, formulas have been obtained for absorption as well as scattering efficiencies.

With this paper of the series, we aim to complete our objective of constructing an analytic framework by the use of which a direct approach to analysis of interstellar dust extinction spectra available for various galaxies *viz.* MW, LMC, SMC etc. can be done very expediently. Whereas, it would be our endeavor to carry out the observed interstellar dust extinction spectra data analysis in context of MW, etc., in a forthcoming paper, nevertheless, a comparison of the extinction produced by equal volumes of PAHs and the two varieties of graphite (perpendicular and parallel) separately is examined here to appreciate the important role of PAHs in shaping the extinction spectra of the dust containing them. The mass density of PAHs and graphite is taken to be the same ($\approx 2.24\text{ gm/cm}^3$) here, as per the general convention so that equal volume also implies equal mass.

The absorption and scattering efficiency data, covering a wide radius range $0.000355\mu m \leq a \leq 0.01\mu m$ and the wavelength range $10\text{\AA} \leq \lambda \leq 10^7\text{\AA}$, for the "astronomical" PAHs

in excellent tabular form can be found on the website of Draine [14]. The details in this regard are available in the appendix part of [9]. These results, to be parametrized in this paper, are referred to as the exact results.

This paper has been organized as follows. Section 2 describes all the relevant functional forms of scattering and absorption efficiencies obtained for PAHs in the wavelength range $1000\text{\AA} \leq \lambda \leq 22,500\text{\AA}$ for size range $5\text{\AA} \leq a \leq 50\text{\AA}$. The accuracy of all the formulas obtained has been demonstrated by numerically computing the absorption and scattering efficiencies from the formulas and contrasting them with the corresponding exact results of Draine [14]. It may be mentioned that the parametrization of these so-called exact results in various wavelength domains have also been achieved by Li and Draine [9]. A typical numerical comparison of their formulas with exact absorption efficiencies has also been presented here in the UV and FUV regions. In section 3, the extinction spectra of various constituents of the carbonaceous component of the dust has been discussed and their relative contributions to the extinction spectrum have been analyzed. The convenience introduced by analytic formalism becomes very apparent in this part of the analysis. The dust model has been described contextually in this section. Finally, we conclude by summarizing and discussing the salient results of this paper in section 4. In this work, grains are assumed to be spheres and, therefore, this work ignores issues related to polarization.

2 Parametrization of PAHs absorption and scattering efficiencies

The computed values of scattering and absorption cross sections of PAHs in the size range $3.5\text{\AA} \leq a \leq 100\text{\AA}$ have been tabulated by Draine [14] for neutral as well as for ionized PAHs in the wavelength range $10\text{\AA} \leq \lambda \leq 10^7\text{\AA}$. We have attempted to obtain simple parametrization for corresponding absorption and scattering efficiencies for PAH sizes $5\text{\AA} \leq a \leq 50\text{\AA}$ for wavelength range $1000\text{\AA} \leq \lambda \leq 22,500\text{\AA}$. The PAHs in this size range have been taken to be the major contributors to the absorption (extinction) due to dust in Li and Draine [9]. Thus, it was decided to restrict the present investigation to the PAH size range $5\text{\AA} \leq a \leq 50\text{\AA}$. The admitted wavelength range is the same as it was in RSG-1 and RSG-2.

For absorption efficiencies, the total wavelength range has been divided into five regions, corresponding to far-ultraviolet ($1000\text{\AA} \leq \lambda < 1800\text{\AA}$), ultraviolet ($1800\text{\AA} \leq \lambda < 4000\text{\AA}$), visible ($4000\text{\AA} \leq \lambda < 8000\text{\AA}$), infrared-I ($8000\text{\AA} \leq \lambda < 12,500\text{\AA}$) and infrared-II ($12,500\text{\AA} \leq \lambda \leq 22,500\text{\AA}$). The corresponding formulas have been accomplished for the neutral as well as the ionic PAHs. Barring region 4 (infrared-I), in each of the other regions, it was

possible to arrive at a single formula covering the entire size range $5 \text{ \AA} \leq a \leq 50 \text{ \AA}$. In the region 4, separate formulas were required for the ranges $5 \text{ \AA} \leq a \leq 10 \text{ \AA}$ and $10 \text{ \AA} \leq a \leq 50 \text{ \AA}$. For the ionic PAHs however, separate formulas are required in regions 3, 4 and 5. In regions 1 (FUV) and 2 (UV), the corresponding absorption efficiency formulas for the neutral and the ionic particles are identical. For scattering efficiencies, we have divided the wavelength range of our interest in three spectral regions. These are far-ultraviolet ($1000 \text{ \AA} \leq \lambda \leq 1800 \text{ \AA}$), ultraviolet ($1800 \text{ \AA} \leq \lambda \leq 4000 \text{ \AA}$) and visible- infrared ($4000 \text{ \AA} \leq \lambda \leq 22,500 \text{ \AA}$).

A parametrization of absorption cross-section of PAHs has also been obtained by Li and Draine [9] starting from the far-ultraviolet to the far-infrared in the size domain $3.5 \text{ \AA} \leq a \leq 100 \text{ \AA}$. Their parametrization is characterized by a set of Drude profiles. Whereas for $\lambda \leq 3300 \text{ \AA}$ the formulas require at most one Drude profile, as many as 12 Drude profiles have been used to construct the formula for $\lambda \geq 3300 \text{ \AA}$.

In this work, numerical comparisons have been generally presented for the values of radius $a = 10, 20, 35$ and 50 \AA . But, it may be mentioned that, in addition, we have also verified all the results for the intermediate values of $a = 5, 8, 15$ and 45 \AA to ensure that all observations and statements made based on them are really speaking valid over the size range $5 \text{ \AA} \leq a \leq 50 \text{ \AA}$.

2.1 Neutral PAHs

In all the formulas to follow, the radius (a) and the wavelength (λ) are in the units of 10^{-5} cm unless stated otherwise. The choice of units is made to confirm with our earlier work (RSG-1 and RSG-2) wherein, the same units are used in the formulas for extinction spectra of the silicate and the graphite particles. The advantage of using these units is to have the numerics associated with $\nu (= 1/\lambda)$ and a as coefficients or in radicals appearing in the various formulas are neither too large, nor too small.

2.1.1 Absorption efficiency

For absorption efficiency, we arrive at the following formulas:

$1000 \text{ \AA} \leq \lambda \leq 1800 \text{ \AA}$ (FUV)

$$Q_{abs}(1) = x \left[\frac{0.93265}{\nu} + \frac{19.608}{\nu} (\nu - 0.643)^2 - \frac{22.2817}{\nu} (\nu - 0.7023)^3 + \frac{6.0}{\nu} (\nu - 0.7023)(1.0 - \nu)(\nu - 0.55) \right], \quad (3.5 \text{ \AA} \leq a \leq 50 \text{ \AA}) \quad (1)$$

where $x = 2\pi a\nu$. Note that the absorption efficiency is proportional to x . This is as it should be. For particles small compared to the wavelength of the incident radiation ($x \ll 1$), the general expression for the absorption efficiency, as a power series in x , is known to be of the form (see, for example, Pendorf [15]):

$$Q_{abs}(x) \approx x(A + Bx^2 + Cx^3 + \dots). \quad (2)$$

where A , B , C etc. are functions of the refractive index of the scatterer relative to the refractive index of the surrounding medium. The minimum and maximum values of x in the present study are 0.000977 (corresponding to $a = 3.5 \text{ \AA}$; $\lambda = 22,500 \text{ \AA}$) and 0.314 (corresponding to $a = 50 \text{ \AA}$; $\lambda = 1000 \text{ \AA}$) respectively. Therefore, in obtaining the formula (1) the first term of the general expression (2) is found to be sufficient in parametrization of the exact absorption efficiency successfully. Higher order terms in x give negligible contribution.

Li and Draine [9] have given two formulas for the absorption efficiency to cover this spectral region which are as follows. For $1000\text{\AA} \leq \lambda \leq 1300\text{\AA}$,

$$Q_{abs} = \frac{a}{100.0(1.286)^3\pi} \left[66.302 - 24.367\nu + 2.950\nu^2 - 0.1075\nu^3 \right], \quad (3)$$

while, for $1300\text{\AA} \leq \lambda \leq 1700\text{\AA}$,

$$Q_{abs} = \frac{a}{100.0(1.286)^3\pi} \left[S_2(\lambda) + 1.8687 + 0.1905\nu + 0.4175(\nu - 5.9)^2 + 0.04370(\nu - 5.9)^3 \right], \quad (4)$$

where S_2 is the particular case ($j = 2$) of the general expression for Drude's spectral absorption profile:

$$S_j(\lambda) \equiv \frac{2}{\pi} \frac{\gamma_j \lambda_j \sigma_{int,j}}{(\lambda/\lambda_j - \lambda_j/\lambda)^2 + \gamma_j^2}. \quad (5)$$

Values of γ_j , λ_j and $\sigma_{int,j}$ are given in [9]. The expressions obtained therein are for absorption cross section per C atom. The corresponding expression for the absorption efficiency is given in the appendix.

$1800\text{\AA} \leq \lambda \leq 5000\text{\AA}$ (UV)

In this wavelength region too, the parametrization of the absorption efficiency could be achieved in a form such that it is proportional to the size parameter x .

$$Q_{abs}(2) = x \left[\frac{1.19}{\nu} - 3.99 \left| 1.0 - \frac{0.462}{\nu} \right| + \frac{1.0}{0.74\nu + 83\nu(1.0 - \frac{0.46}{\nu})^2} \right], \quad (3.5\text{\AA} \leq a \leq 50\text{\AA}) \quad (6)$$

The formulas obtained in [9] for this region are:

$$Q_{abs} = \frac{a}{100.0(1.286)^3\pi} \left[S_2(\lambda) + 1.8687 + 0.1905\nu \right], \quad (7)$$

for $1700\text{\AA} \leq \lambda \leq 3030\text{\AA}$, and

$$Q_{abs} = \frac{a}{100.0(1.286)^3\pi} \left[34.58 \times 10^{-3.431/\nu} \text{cutoff}(\lambda, \lambda_c) + \sum_{j=3}^{14} S_j(\lambda) \right], \quad (8)$$

for $\lambda \geq 3030\text{\AA}$, where S_j is given by equation (5). It may be noted that $\text{cutoff}(\lambda, \lambda_c)$ is a function of a as well as λ because λ_c is a function of the radius a of the PAH particle [9].

$4000\text{\AA} \leq \lambda \leq 8000\text{\AA}$ (Visible)

$$Q_{abs}(3) = x \left[(28.176\nu^2 - 0.091\nu - 0.311) - (a - 0.048)^2 (4600\nu^2 - 2052.66\nu + 226.26) \right] - \frac{(0.041/100a)^{5/2}}{1 + (2175a)^3 \left[0.1228 + \frac{0.01312}{(100a)^2} - \nu \right]^2} - \left(1.3 - \frac{1}{4\nu} \right) \left(\frac{0.00355}{10a} \right)^3, \quad (5\text{\AA} \leq a \leq 50\text{\AA}) \quad (9)$$

Figure 1(a) shows a comparison of absorption efficiencies computed on the basis of our formulas with the exact results [14] for four PAHs sizes. The wavelength range is 1000\AA to 8000\AA .

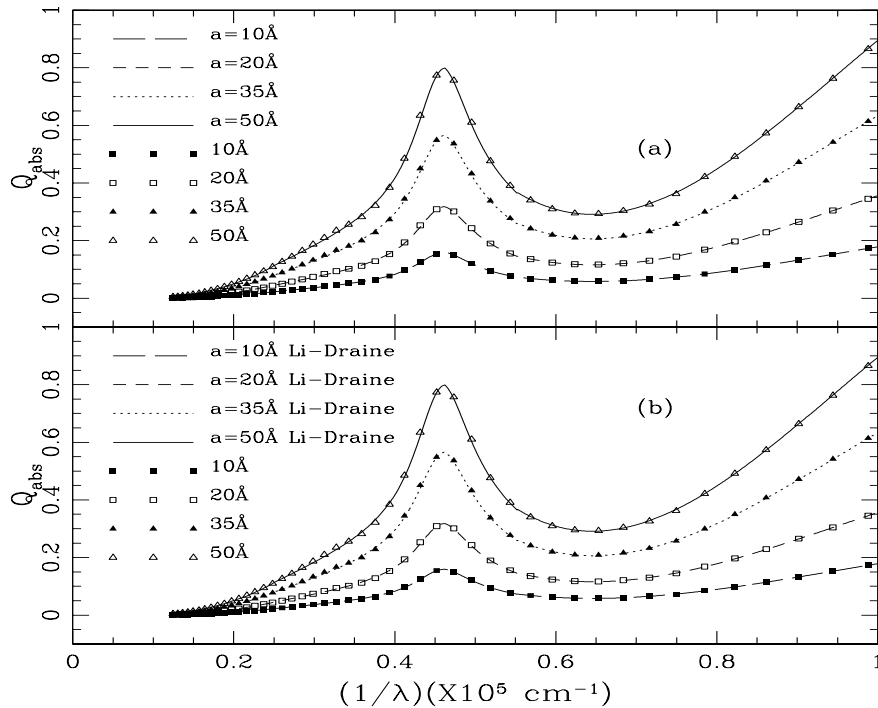


Fig1 (a): Comparison of predictions (lines) of absorption efficiencies from our equations with exact results (Draine website[8]) points

(b): Comparison of predictions (lines) of absorption efficiencies from Li and Draine 2001 equations with exact results (Draine website[8]) points

Frequency range $0.125 \leq \nu \leq 1.0$, wavelength range $1000\text{\AA} \leq \lambda \leq 8000\text{\AA}$ (i.e. FUV+UV+Visible region)

It can be seen that the agreement between the predictions of (1) and (6) and the exact results is excellent. To contrast results from formulas (1) and (6) with those from the

parametrization by Li and Draine [9], a typical comparison of absorption efficiencies computed from formulas (3), (4), (7) and (8) with exact results is shown in Figure 1(b). Clearly, the accuracy of Li and Draine parametrizations and our formulas is almost identical.

8000Å ≤ λ ≤ 12,500Å (Infrared- I)

$$Q_{abs}(4) = \frac{a[0.01391 + a(3.1296 - 32.3a)]}{1.0 + [113.3 + (10.43 - \frac{0.27}{a})^2](\frac{0.1245}{\nu} - 1.0)^2} + \frac{(0.00422/100a)^2}{1.0 + (10\nu - 0.8)^2},$$

$$(10\text{\AA} \leq a \leq 50\text{\AA}) \quad (10a)$$

$$Q_{abs}^s(4) = \frac{0.00208a}{1.0 - 2.4[0.22 + a(94.0 + C)](1.0 - \frac{0.00644}{\nu^2})^2} + \left(\frac{0.00117}{a}\right)^4 (\nu - 0.08)(0.1245 - \nu),$$

$$(5\text{\AA} \leq a \leq 10\text{\AA}) \quad (10b)$$

where

$$C = 438(1.0 - 100a)(100a - 0.5)^2.$$

and the superscript s in (10b) stands for small PAH range $5\text{\AA} \leq a \leq 10\text{\AA}$. Figure 2(a) exhibits a comparison of variation of absorption efficiency computed on the basis of (10a) with exact results. For clarity of display, the comparison has been shown only for two values of PAH sizes, $a = 20\text{\AA}$ and $a = 50\text{\AA}$. The agreement can be seen to be excellent. Although not shown here, computations have been done for (10b) also and the results have been found to agree reasonably well with exact results.

It appears that the molecular structure of PAHs become vital in this wavelength range, for the absorption does not seem to follow the general expression (6) which is obtained from the expansion of Mie formulas for small x values.

12,500Å ≤ λ ≤ 22,500Å (Infrared- II)

$$Q_{abs}(5) = 0.01x \left[\frac{\sqrt{\nu}}{1.0 + (1000a - 50.0)^4} + 3\nu(1.0 + 2.2a) + 0.168 - 0.2a \right], \quad (5\text{\AA} \leq a \leq 50\text{\AA})$$

$$(11)$$

A comparison of absorption efficiencies computed from (11) with exact results is depicted in Figure 2(b). Once again, the agreement of our formula with exact results is excellent.

Above comparisons show that our formulas for absorption efficiency give excellent results over the entire wavelength and size range considered here. Formulas obtained involve only frequency of radiation and the size of the scatterer and are simple to use. In contrast,

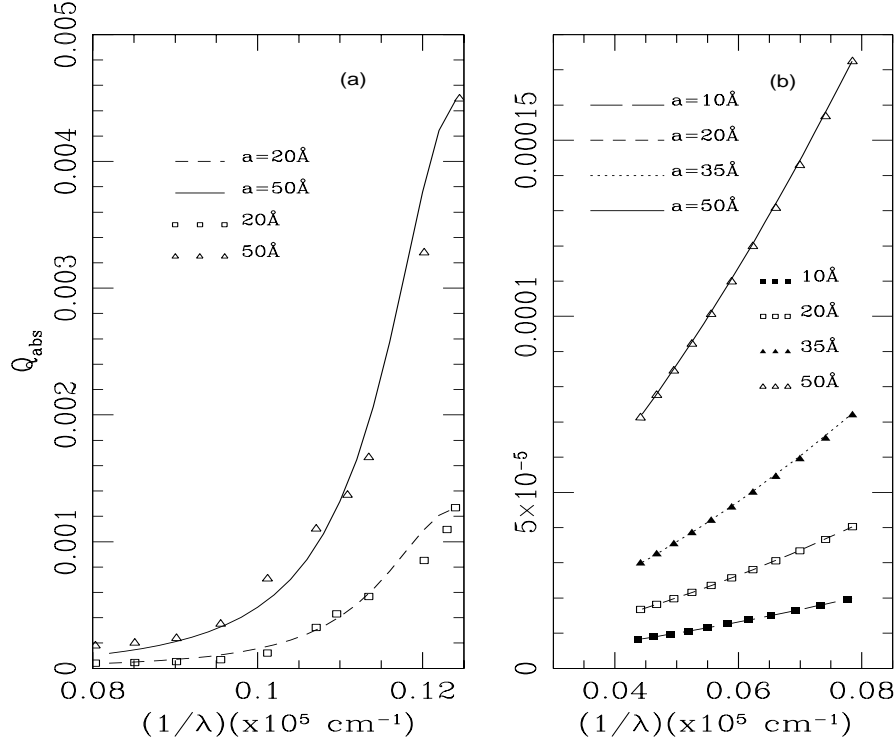


Fig 2: Comparison of predictions (lines) of absorption efficiencies of our equations with exact result (Draine's website [8]) points

(a): Frequency range $0.08 \leq \nu \leq 0.125$; wavelength range $8000\text{\AA} \leq \lambda \leq 12,500\text{\AA}$ (IR-1)

(b): Frequency range $0.044 \leq \nu \leq 0.08$; wavelength range $12,500\text{\AA} \leq \lambda \leq 22,500\text{\AA}$ (IR-2)

the Li and Draine formulas [9], for $\lambda \geq 3000\text{\AA}$, require contributions from as many as 12 Drude profiles making it somewhat cumbersome to use fluently. The formula also involves a function $\text{cutoff}(\lambda, \lambda_c)$ containing the cutoff wavelength λ_c which in turn, depends on the PAH radius in a complex manner.

2.1.2 Scattering efficiencies

For the scattering efficiencies, the formulas for the neutral or the ionic PAHs turn out to be identical. These are as follows.

$1000\text{\AA} \leq \lambda \leq 1800\text{\AA}$ (FUV)

$$Q_{\text{sca}}(1) = x^4 \left[\frac{0.112}{\nu^2} + 9.8 \left(1.0 - \frac{0.620}{\nu} \right)^2 + \frac{36.124}{\nu^2} \left(1.0 - \frac{0.657}{\nu} \right)^4 + x^2 \left(\frac{\nu}{0.507\nu + 34.0(1-\nu)^2} - \frac{x}{1.96 + 2.665\nu - 4.2\nu^2} \right) + \frac{0.09}{[1.0 + (40\nu - 38.0)^2]^2} \right], \quad (5\text{\AA} \leq a \leq 50\text{\AA}) \quad (12)$$

$$1800\text{\AA} \leq \lambda \leq 4000\text{\AA} \text{ (UV)}$$

$$Q_{sca}(2) = x^4 \left[\frac{1.0}{\nu(0.4485 + 157.0\nu^2(1 - \frac{\nu}{0.4562})^2)} + \frac{0.25}{1 + (50\nu - 16)^2} \right]. \quad (5\text{\AA} \leq a \leq 50\text{\AA}) \quad (13)$$

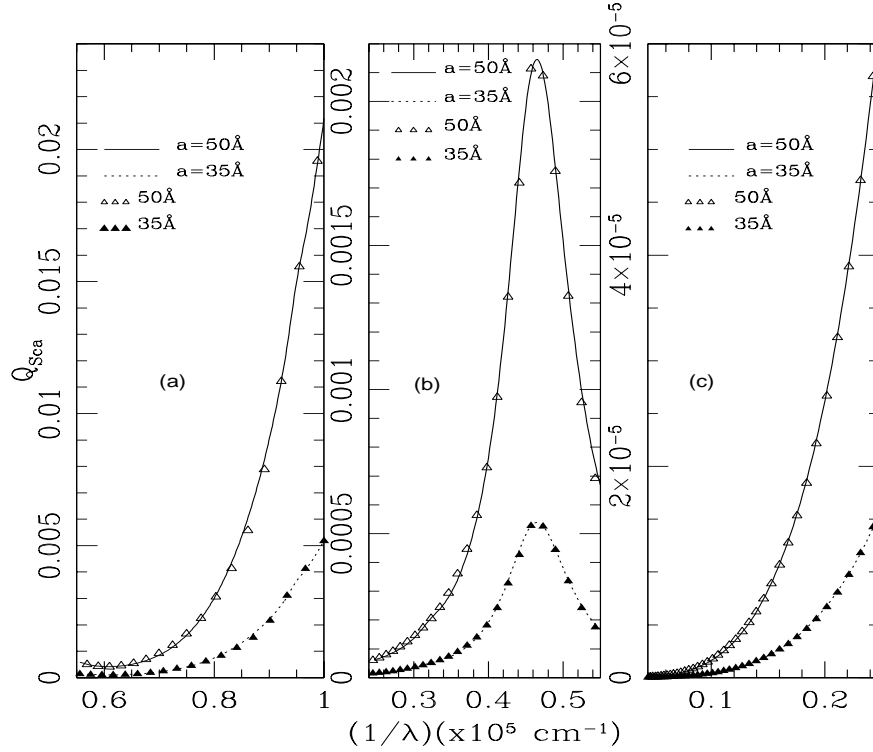


Fig 3: Comparisons of predictions (lines) of scattering efficiencies from our equations with the exact results (Draine's website [8]) points

(a): Frequency range $0.55 \leq \nu \leq 1.0$; wavelength range $1000\text{\AA} \leq \lambda \leq 1800\text{\AA}$ (FUV)

(b): Frequency range $0.25 \leq \nu \leq 0.55$; wavelength range $1800\text{\AA} \leq \lambda \leq 4000\text{\AA}$ (UV)

(c): Frequency range $0.044 \leq \nu \leq 0.25$; wavelength range $4000\text{\AA} \leq \lambda \leq 22,500\text{\AA}$ (Visible+IR)

$$4000\text{\AA} \leq \lambda \leq 22,500\text{\AA} \text{ (Visible, IR-I, IR-II)}$$

$$Q_{sca}(3) = 1.66 x^4, \quad (5\text{\AA} \leq a \leq 50\text{\AA}) \quad (14)$$

The functional forms of the scattering efficiency in these spectral regions may be contrasted with the expansion of exact Q_{sca} in powers of x for small x (see, for example, Pendorf [15]):

$$Q_{sca}(x) \approx x^4(D + Ex^2 + Fx^3 + \dots) \quad (15)$$

where D , E , F etc. are effectively, functions of the refractive index. It may be noted that while for (13) and (14) only the first term (of the order of x^4) is sufficient to reproduce the observed results, for (12) the second and the third terms, of the order of x^6 , x^7 are also required.

2.2 Ionic PAHs

In the wavelength regions 1 and 2 (FUV, UV) the formulas remain the same as that for non-ionic PAHs. For the other three regions (Visible, IR-I, IR-II), following formulas have been obtained for the absorption efficiencies,

4000Å ≤ λ ≤ 8000Å (Visible)

$$Q_{iabs}(3) = x \left[28.176\nu^2 - 0.091\nu - 0.311 - (a - 0.048)^2(4600\nu^2 - 2052.66\nu + 226.26) - \frac{(0.4858/100a)^4}{1.0 + 20.0(100\nu - 14.3)^2} \right] + \frac{0.0006(0.01/a)^3}{1.0 + 0.20(100\nu - 13.4)^4}, \quad (10\text{\AA} \leq a \leq 50\text{\AA}) \quad (16a)$$

$$Q_{iabs}^s(3) = a\nu(178.568\nu^2 - 2.184) - \frac{0.0005(0.005/a)^3}{1.0 + 7(100\nu^2 - 1.96)^2}, \quad (5\text{\AA} \leq a \leq 10\text{\AA}) \quad (16b)$$

8000Å ≤ λ ≤ 12,500Å (Infrared- I)

$$Q_{iabs}(4) = \frac{0.1a - 0.0001}{1.0 + \left[68.0 + \frac{0.41}{a} + 37.55 \left(\frac{0.0207}{a} - 1.0 \right)^3 \right] \left(\frac{0.1245}{\nu} - 1.0 \right)^2}, \quad (10\text{\AA} \leq a \leq 50\text{\AA}) \quad (17a)$$

$$Q_{iabs}^s(4) = \frac{0.21a - 0.001077 - 0.01(100a - 0.768)^3}{1.0 + \left[\frac{0.90}{a} + \frac{28.0}{\sqrt{a}} \left| 1.0 - \frac{0.0071}{a} \right| \right] \left(\frac{0.1245}{\nu} - 1.0 \right)^2} + \frac{(3.425 - 25\nu)(0.005/100a)^2}{10.0 + 3 \left(10.0 - \frac{0.89}{\nu} \right)^2}, \quad (5\text{\AA} \leq a \leq 10\text{\AA}) \quad (17b)$$

12,500Å ≤ λ ≤ 22,500Å (Infrared- II)

$$Q_{iabs}(5) = Q_{abs}(5) + a \left[(0.005)^2 + 0.116(\nu - 0.0675)^2 \right] + \frac{0.00352a - (0.04134 - a)^3}{1.0 + \left[\frac{0.22}{a} \left(\frac{0.89}{\nu} - 10 \right)^4 \right]}, \quad (10\text{\AA} \leq a \leq 50\text{\AA}) \quad (18a)$$

$$Q_{iabs}^s(5) = a(0.3\nu^2 - 0.00434\nu + 0.000532), \quad (5\text{\AA} \leq a \leq 10\text{\AA}) \quad (18b)$$

where the subscript *iabs* used in *Q* indicates absorption efficiency for ionic PAHs. In the far-ultraviolet and ultraviolet regions, the absorption and scattering efficiencies for neutral and ionic PAHs are identical. They, however, differ in visible and infrared regions as can be seen from Figure 3 which depicts this difference for $a = 10\text{\AA}$ and $a = 50\text{\AA}$. The curves have been plotted using above formulas. The curves show that the absorption by the ionic PAHs is generally greater in comparison to the neutral PAHs. More recently, Cecchi-Pestellini [16] have reported on variation of spectral properties of PAHs in various charged states. However,

in the present work we limit ourselves only to the gross classification of neutral and charged PAHs, which is sufficient for our purposes. Scattering of electromagnetic radiation by a charged sphere has been treated by Klacka and Kocifaj [17] employing a generalization of the Mie theory.

3 Extinction spectral features of PAHs

Having obtained the absorption and scattering efficiency formulas in the various frequency ranges, one can generate the extinction spectra for PAHs for a specified particle concentration N_{PAH} and a size distribution function $f_p(a)$ over a radius range $[a_0, a_m]$: $5\text{\AA} \leq a_0$, $a_m \leq 50\text{\AA}$ using the expression:

$$K_{ext}(\lambda) = \frac{\pi N_{PAH}}{10^{10}} \int_{a_0}^{a_m} Q_{ext}^{PAH}(x) a^2 f_p(a) da, \quad (19)$$

$f_p(a)$ being normalized to unity. In (19), $Q_{ext}^{PAH}(x) = Q_{abs}^{PAH} + Q_{sca}^{PAH}$ is the extinction efficiency of an individual scatterer of size parameter $x = 2\pi a/\lambda$; a and λ being reckoned in unit 10^{-5} cm. This choice of units is in keeping with our earlier formulas for extinction spectra of silicate and graphite grains expressed in [1,2]. It may be observed that $Q_{sca}^{PAH} \ll Q_{abs}^{PAH}$ in the wavelength and radius ranges considered here. Hence, in (19) one can simply use Q_{abs}^{PAH} in the place of Q_{ext}^{PAH} without incurring appreciable error.

The K_{ext} spectra (19) assumes much simpler form in the wavelength region where Q_{abs}^{PAH} is linear in a . We observe that such is the case with the FUV and UV regions. In each of these regions we have $Q_{ext}^{PAH} \approx a\phi(\nu)$. As a result, the corresponding expression for K_{ext}^{PAH} in the wavelength region $1000\text{\AA} \leq \lambda \leq 5000\text{\AA}$ is given by the simple form

$$K_{ext}^{PAH}(\lambda) \approx \frac{\pi N_{PAH}}{10^{10}} \overline{a^3}_{PAH} \phi(\nu), \quad (20)$$

The volume corresponding to N_{PAH} number of particles will be

$$V_{PAH} = \frac{4\pi}{3} N_{PAH} \overline{a^3}_{PAH} \times 10^{-15}, \quad (21)$$

where

$$\overline{a^3}_{PAH} = \int_{a_0}^{a_m} a^3 f_p(a) da,$$

a , a_0 , a_m all are in 10^{-5} cm. units. Using (21) in (20), we finally have,

$$K_{ext}^{PAH}(\lambda) \approx \frac{3 \times 10^5}{4} V_{PAH} \phi(\nu). \quad (22)$$

In the other wavelength regions covering $5000\text{\AA} \leq \lambda \leq 22,500\text{\AA}$, however, the K_{ext}^{PAH} spectra would be dependent on the size distributional details in more involved manner rather than

simply being proportional to the third moment $\overline{a^3}$ as seen in (20).

If a population of PAHs specified by N_{PAH} , $f_p(a)$ and V_{PAH} is included in the carbonaceous matter sector alongside graphite parallel as well as perpendicular components then due to stronger absorption features in the FUV and UV regions, a smaller amount of PAH (as compared to graphite) has the ability to increase the extinction contribution of the carbonaceous component of the dust by much larger amount. As a result, when one has to include a population of PAHs to any silicate-graphite model (two-component MRN model) in a manner so that the relative mass abundance criterion (silicate mass/ carbonaceous mass) is maintained while the desired changes in the dust (PAHs + silicate + graphite) extinction spectra are obtained, one can concentrate mainly to the FUV and UV regions. Thus among many, a simple option while extending a two-component silicate-graphite model would be to replace a definite amount of existing graphite (by mass) with equal amount (by mass) of PAHs. Taking the mass density ($\approx 2.24 \text{ gm/cm}^3$) to be the same for both graphite and PAHs in bulk, we are thus led to a comparative study of the extinction spectra produced by equal volumes of graphite grains (parallel, perpendicular) and the PAHs. In the following, we examine this point in some details with respect to the MRN model considered by us in [1,2].

It may be recalled that in the two component graphite-silicate model of Mathis et al. (1979) [18], the spherical grains (graphite as well as silicate) are taken to follow a power-law size distribution of the form:

$$f(a) \propto a^{-3.5} \quad a_0 \leq a \leq a_m, \quad (23)$$

where, a is the radius of the grain varying within the chosen values of a_0 and a_m . Besides, graphite material is taken to be present in two distinct structural varieties within the specified range of a_0 and a_m . This plausibility lies in the fact that graphite is a highly anisotropic material. The refractive index of graphite, therefore, depends on the orientation of electric field relative to its structural symmetry. Owing to practical difficulties in calculations of exact scattering (extinction) quantities due to the anisotropy, researchers have taken resort to an approximation known as “ $\frac{1}{3} - \frac{2}{3}$ ” approximation [19]. In this approximation, graphite grains are represented as a mixed population of isotropic spheres, of which $\approx \frac{1}{3}$ fraction have refractive index $m = m_{\parallel}$ (referred to as graphite parallel) and $\approx \frac{2}{3}$ fraction have the refractive index $m = m_{\perp}$ (referred to as graphite perpendicular). By virtue of [1,2], we have formulas for generating graphite extinction spectra for both the components (graphite perpendicular and graphite parallel) within the parameter ranges

$$0.002\mu m \leq a_0 \leq 0.05\mu m; \quad 0.15\mu m \leq a_m \leq 0.25\mu m.$$

By choosing $N_{gra} = 4.4 \times 10^8$ as the particle concentration for both varieties of graphite (perpendicular as well as parallel) and the size range $[0.005\mu m : 0.25\mu m]$, the corresponding extinction spectra are displayed in Figure 4(b).

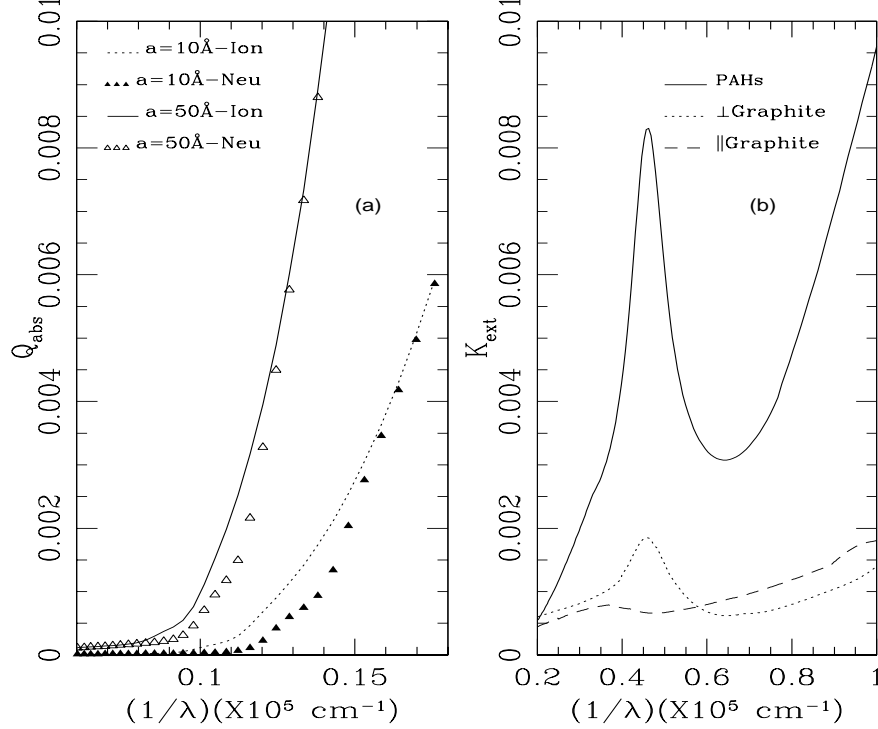


Fig 4 (a): Comparison of predictions of absorption efficiencies of Neutral and Ionic PAH's.
(b): Extinction spectra for equal volumes of PAH's and, parallel and perpendicular graphite grains.

The associated material volume of each of the graphite components is $V_{gra} = (4\pi/3) N_{gra} \overline{a^3}_{gra} \times 10^{-15} \text{cc}$, $\overline{a^3}_{gra}$ being the mean cube radius of the corresponding population of graphite particles. The radius a has units in 10^{-5}cm ; $\overline{a^3}_{gra}$ is to be evaluated using the formula [1]

$$\overline{a^3}_{gra} = 5a_0^3(n-1) \left(1 - \frac{1}{n^5}\right)^{-1}, \quad (24)$$

with $a_0 = 0.05$; $a_m = 2.5$ and $n^2 = (a_m/a_0) = 50$.

If we have to generate the PAHs extinction spectra corresponding to an equal bulk of graphite (perpendicular or parallel) having this fixed volume V_{gra} we must use this value for V_{PAH} occurring in (22). The resultant PAHs extinction spectrum is also displayed in Figure 4(b) along with that of the two graphite components bringing out the contrast in the individual extinction spectra produced by equal volumes of PAHs and the two varieties of graphite. It is clear from Figure 4(b) that the contribution of some mass of PAHs to the interstellar dust extinction will be much greater in comparison to equal mass of graphite in the wavelength range $1000\text{\AA} \leq \lambda \leq 5000\text{\AA}$ (FUV and UV regions). Further, if one looks at

the ratio $K_{ext}(\lambda)/K_{ext}(\lambda_v)$ fixing λ_v at 5000\AA and compares among the three species viz. PAHs, graphite (perpendicular) and graphite (parallel), one can see easily that the ratio is much greater for PAHs as compared to that of the other two species within the wavelength range 1000\AA to 5000\AA . Clearly, replacement of a small amount of graphite by an equal amount of PAHs in a dust mixture will cause an increase in the dust extinction throughout the wavelength range 1000\AA to 5000\AA . However, this increase would be greater in the FUV region than that in the UV region. This is how the addition of PAHs to silicate-graphite model will help one to adjust the interstellar dust extinction spectral features in the FUV, UV regions.

In connection with our choice for the PAHs grain size range, we would like to mention that, in Li and Draine [9] size range of PAHs has been taken to be $0.00035 \leq a \leq 0.01 \mu m$ in their investigations. The absorption cross section of carbonaceous grains is represented as [9]

$$\begin{aligned} C_{abs}^{carb}(a, \lambda) &= \xi_{PAH} C_{abs}^{PAH}(a, \lambda) + (1 - \xi_{PAH}) C_{abs}^{gra}(a, \lambda), \\ \xi_{PAH}(a) &= (1 - q_{gra}) \times \min[1, (a_\xi/a)^3], \\ a_\xi &= 50\text{\AA}, \quad q_{gra} = 0.01, \end{aligned}$$

where C_{abs}^{PAH} , C_{abs}^{gra} are, respectively, absorption cross-sections of PAH and graphite grains of radius a and wavelength λ ; a_ξ is the grain radius from which the transition from PAH properties to graphite properties begins; ξ_{PAH} is the PAH weight factor which falls off continually as a increases from a_ξ to infinity. However, as has been mentioned in [9], this choice of the weight factor is quite arbitrary. With this freedom of choice for ξ_{PAH} , we consider a dust model in which the carbonaceous component is made up of PAHs of size range $5\text{\AA} \leq a \leq 50\text{\AA}$ and graphite grains in the size range $0.005\mu m \leq a \leq 0.25\mu m$.

4 Conclusions and discussions

In this work, we have analyzed the extinction spectra generated by small size carbonaceous matter present in interstellar dust in the form of Polycyclic Aromatic Hydrocarbons (PAHs). Our investigations cover the wavelength region $1000\text{\AA} \leq \lambda \leq 22,500\text{\AA}$ with PAHs size range $5\text{\AA} \leq a \leq 50\text{\AA}$, a being the radius of the PAH particle. In doing so, we have made use of the scattering and absorption efficiency data available in [14] to obtain simple and accurate analytic formulas for scattering and absorption efficiencies expressible as functions of a and λ . These formulas can be used expediently for computing extinction spectra generated by some bulk PAHs material specified through any selected size distribution. Thus, this work, together with our earlier work [1,2] essentially completes our search for an analytic platform for interstellar dust extinction spectra analysis which employ MRN type dust models containing silicate, graphite and PAHs as well.

The scattering efficiency has $(a/\lambda)^4$ behavior over $1800\text{\AA} \leq \lambda \leq 22,500\text{\AA}$. For $1000\text{\AA} \leq \lambda \leq 1800\text{\AA}$, the behavior is slightly different in that additional $(a/\lambda)^6$ and $(a/\lambda)^7$ behavior also creeps in. This is quite in keeping with the Pendorf formula [15] for the scattering efficiency in the case of small values of a/λ . The absorption efficiency has a/λ behavior over $1000\text{\AA} \leq \lambda \leq 5000\text{\AA}$ which is again in keeping with the Pendorf formula for absorption efficiency in respect of small values of a/λ . However, for $\lambda \geq 5000\text{\AA}$ sharper absorption features characterizing the special dispersive properties depending on size of the particle appear. This results in the absorption efficiency having a functional form which differs from that of Pendorf. A good account of modelling for these sharper absorption features occurring in the extinction spectra data experimentally generated by small sized hydrocarbons prepared in the laboratory is given by Li and Draine [9].

The ionic PAHs show a slightly different extinction behavior as compared to their neutral counterparts. Both the neutral and the ionic species have the same scattering efficiencies and hence scattering properties of these are exactly the same within the size range $3.5\text{\AA} \leq a \leq 50\text{\AA}$ and the wavelength range $1000\text{\AA} \leq \lambda \leq 22,500\text{\AA}$. The neutral and the ionic PAHs absorption efficiencies are same for $1000\text{\AA} \leq \lambda \leq 4000\text{\AA}$; but they differ in the wavelength range $4000\text{\AA} \leq \lambda \leq 22,500\text{\AA}$. The pattern of variation is illustrated in Figure 4(a). One can see that the range of wavelength $[\lambda_1, \lambda_2]$ over which the absorption efficiency differs depends on the PAH radius a . It appears that both λ_1 and λ_2 increase with a . As the efficiency differences are not substantial, the preference of ionic over neutral PAHs to be included in the dust model does not seem to provide with much changes in the corresponding extinction spectra.

To estimate the extent to which the extinction spectra of a dust can be affected by having a definite amount of PAHs in it, we have compared the extinction spectra generated by equal volumes of all the three carbonaceous components viz, graphite (perpendicular), graphite (parallel) and PAHs. As PAHs extinction is essentially due to absorption only, we have chosen the wavelength range $1000\text{\AA} \leq \lambda \leq 5000\text{\AA}$ due to the simple form of the absorption efficiency. The comparison brings out very clearly the fact that PAHs indeed can act as a very effective carbonaceous component in MRN type dust models. It will be our future endeavor to use the analytic framework which includes this work alongside [1,2] for the analysis of extinction spectra data corresponding to MW, LMC and SMC.

Appendix

The absorption cross section per C atom has been denoted in [9] as C_{abs}^{PAH}/N_C , where N_C is the number of C atoms. The absorption efficiency, Q_{abs}^{PAH} , for a PAH of size a can be expressed as

$$Q_{abs}^{PAH}(a, \lambda) = \frac{N_C}{\pi a^2} C_{abs}^{PAH} / N_C$$

The “radius” a of a PAH containing N_C number of C atoms is defined to be the radius of a sphere with carbon density of graphite containing the same number of C atoms, i.e., $a = 1.286 N_C^{1/3}$. Thus,

$$Q_{abs}^{PAH}(a, \lambda) = \frac{a}{\pi(1.286)^3} C_{abs}^{PAH} / N_C,$$

where C_{abs}^{PAH}/N_C is given in equations (5)-(11) in [9] for various spectral ranges.

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